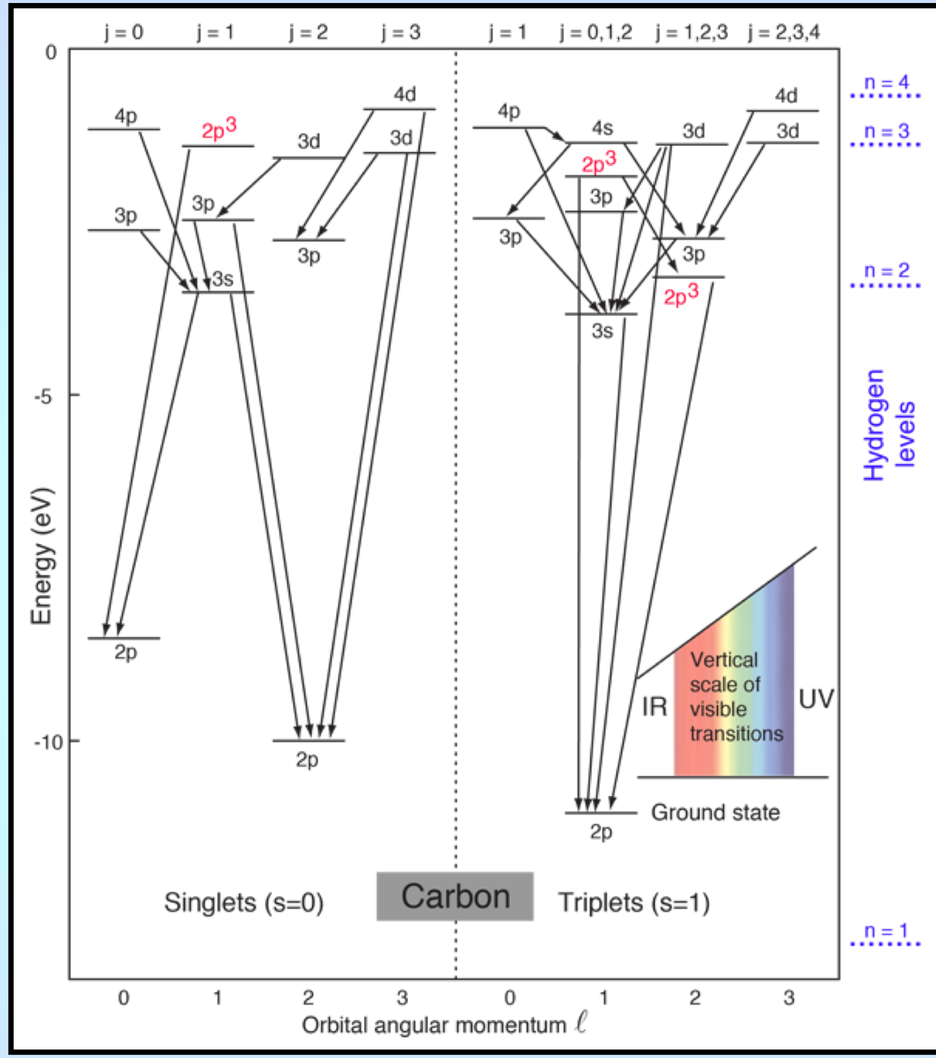
Electron and Atomic Quantum Numbers

Every state in an atom is defined by 4 quantum numbers: the principle quantum number (*n*), the orbital angular momentum (*l*), the magnetic quantum number (*m*), and the electron spin (*s*), which is ±½ in the up or down direction.

If you add up (vectorially), all the orbital angular momenta of all the atom's electrons, you get the total orbital angular momentum of the atom, *L*. These have the same letters as for the orbitals (*s*=0, *p*=1, *d*=2, *f*=3, etc.), except the letters are capitalized (*S*, *P*, *D*, *F*, etc.)

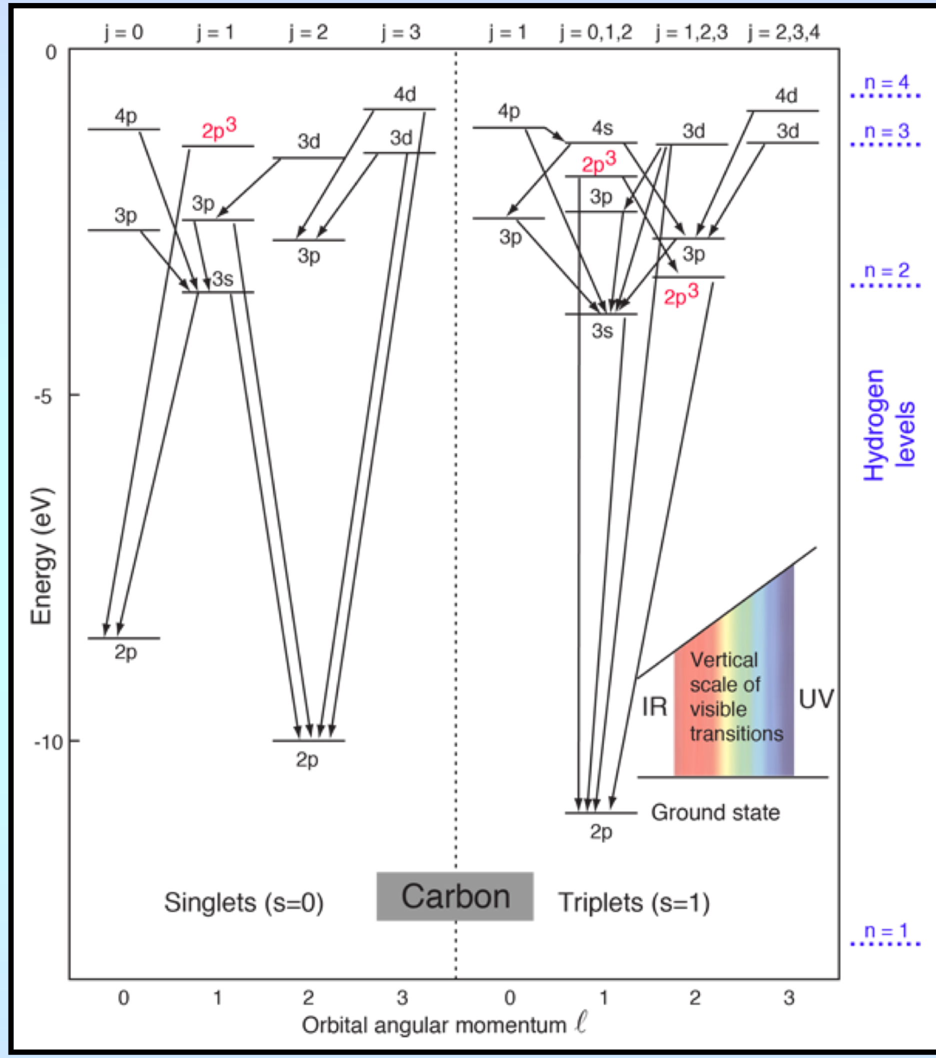


Electron and Atomic Quantum Numbers

Every state in an atom is defined by 4 quantum numbers: the principle quantum number (n), the orbital angular momentum (l), the magnetic quantum number (m), and the electron spin (s), which is ±½ in the up or down direction.

Similarly, if you add up all the electron spins (vectorially), you get the atom's total electron spin, S. And, you add up (vectorially) all the orbital and spin angular momentum, you get the total angular momentum of the atom, J.

(Note: complete shells always sum to zero.)



$$L = \sum_i \vec{\ell}_i \qquad S = \sum_i \vec{s}_i \qquad \vec{J} = \vec{L} + \vec{S}$$

(sort of)

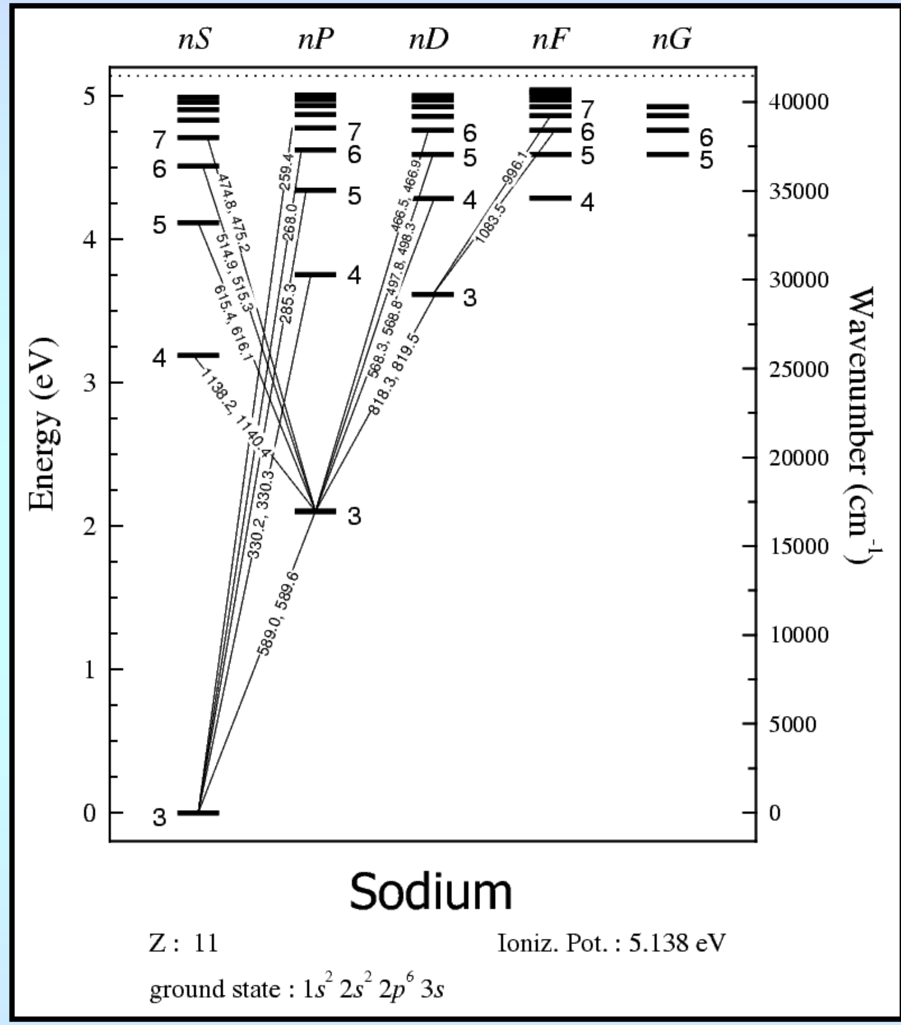
Statistical Weight and Spectroscopic Notation

An atom generally doesn't care about its orientation. As a result, there can be multiple states with the same L and S, but different J values. In this case, as all the J levels have exactly the same energy, we can treat them as one level, but give that level a "statistical weight" equal to the number of separate states, i.e.,

$$\omega = (2J+1) = (2L+1)(2S+1)$$

In spectroscopic notation, one writes an energy level as

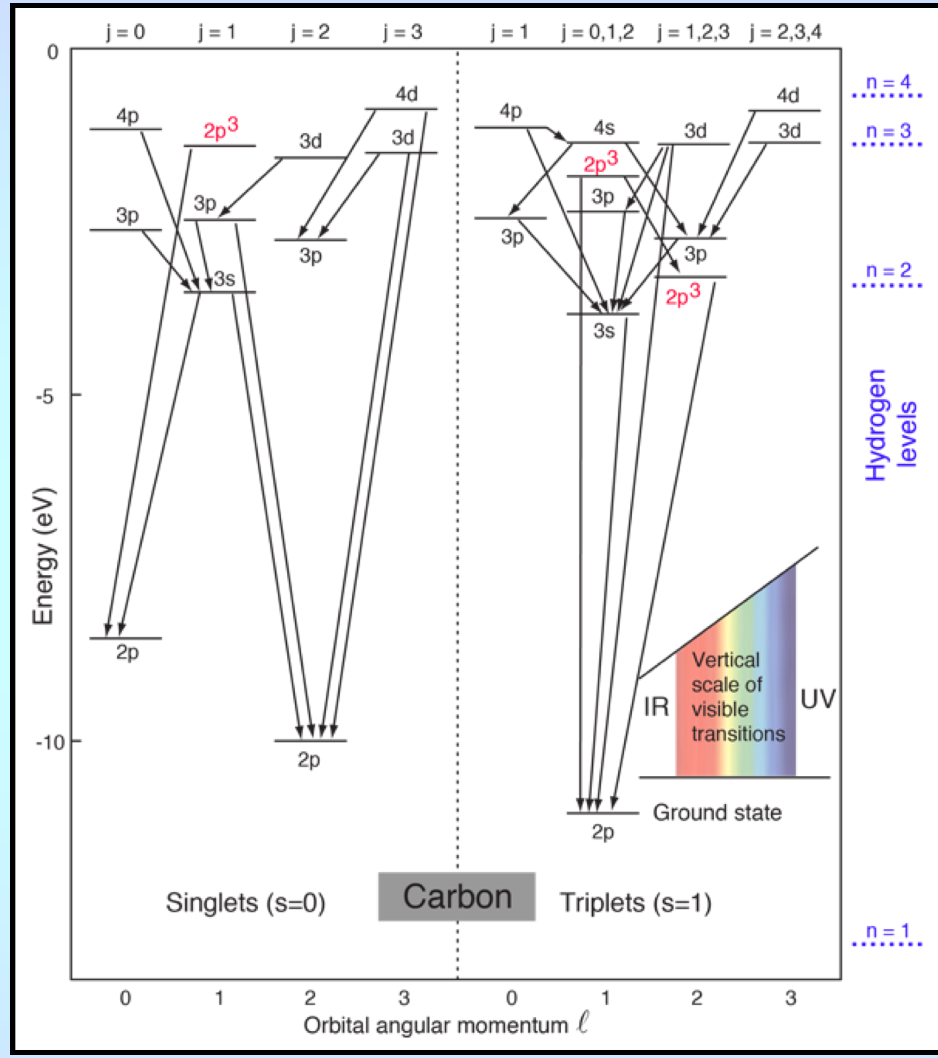
$$^{(2S+1)}L_J$$



where S is the total (vectoral) electron spins, L is their total (vectoral) orbital angular momentum and J is the total (vectoral) momentum.

Electron Transitions

Not all transitions in an atom are equally likely. If n changes, $\Delta J = -1, 0$, or $+1$ (but not $J=0$ to $J=0$) and $\Delta S=0$, then the transition is extremely likely, i.e., "permitted". Effectively, this means $L' = L \pm 1$. If such selection rules are violated, then the transition is "forbidden".



The Einstein A values give the precise likelihood of a transition: the higher the A value, the more likely it is to occur.

(FYI: the probability of an absorption is directly proportional to this A value.)

Permitted transitions have $A \gtrsim 10^5$ sec^{-1} (i.e., they will typically occur within $\sim 10^{-5}$ sec); forbidden transitions have $A \lesssim 1$ sec^{-1}.

Transition Rates

There are actually 3 Einstein coefficients. For level $i > j$

$A_{i,j}$: the spontaneous emission coefficient

$B_{i,j}$: the induced emission coefficient (for stimulated emission)

$B_{j,i}$: the absorption coefficient

These coefficient are related:

$\omega_i B_{i,j} = \omega_j B_{j,i}$ and $$A_{i,j} = \frac{2h\nu^3}{c^2}\frac{\omega_j}{\omega_i}B_{j,i}$$

In general, the larger the energy difference of a permitted transition, the larger its A value, with $A \propto \nu^3$.

Aside: Transition Rates and Oscillator Strengths

Analyses of emission line strengths require a knowledge of the Einstein A values. But most astronomers who analyze the absorption lines in stellar atmospheres perfer to describe the strengths of atomic transitions via the line's oscillator strength, *f*. The two are related by

$$A_{i,j} = \frac{2\pi\nu^2 e^2}{\epsilon_0 m_e c^3} \frac{\omega_j}{\omega_i} f_{j,i}$$

$$B_{j,i} = \frac{e^2}{4\epsilon_0 m_e h\nu} f_{j,i}$$

$$B_{i,j} = \frac{e^2}{4\epsilon_0 m_e h\nu} \frac{\omega_j}{\omega_i} f_{j,i}$$

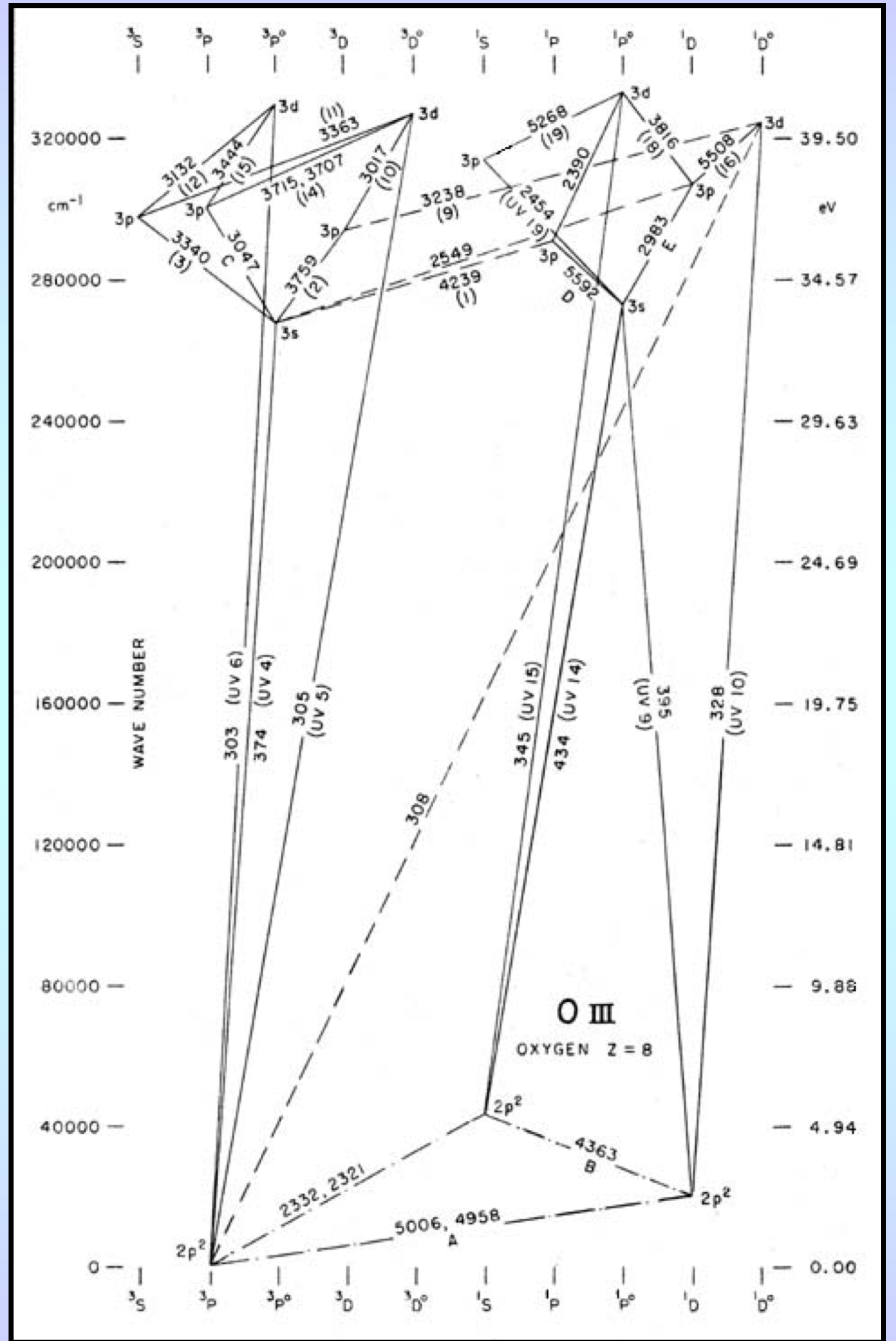
where e is the charge of the electron and ε_0 is the permittivity of free space ($\varepsilon_0 = 1$ in cgs units).

An Example

In the ISM, elements may be in several ionization states. Neutral species are designated by a superscript “0” or the Roman numeral I. For example,

- neutral oxygen is O^0 or O I.
- Ionized oxygen is O^+ or O II.
- Doubly-ionized oxygen is O^{++} or O III.

And so on.



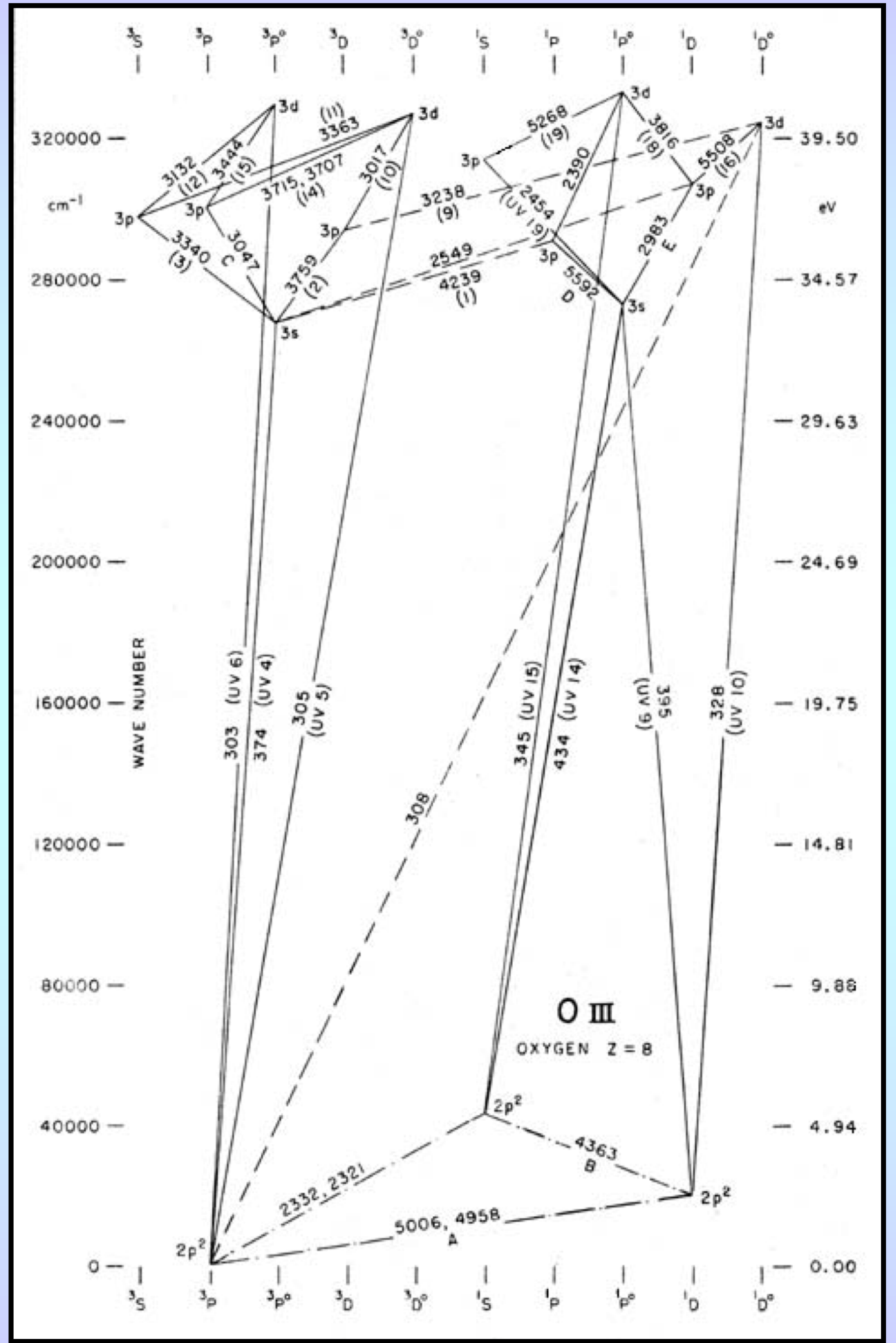
An Example

The A-value of the 5007 Å line of O^{++} is $A = 0.02\ \mathrm{sec}^{-1}$; it takes so long to decay that it is impossible to observe in a laboratory, as the electron is much more likely to have a collision before decaying.

However, in the ISM, the density is so low that this not problem. This line is *extremely* common.

The 5007 Å line was originally called “nebulium”, since it was only seen in nebulae.

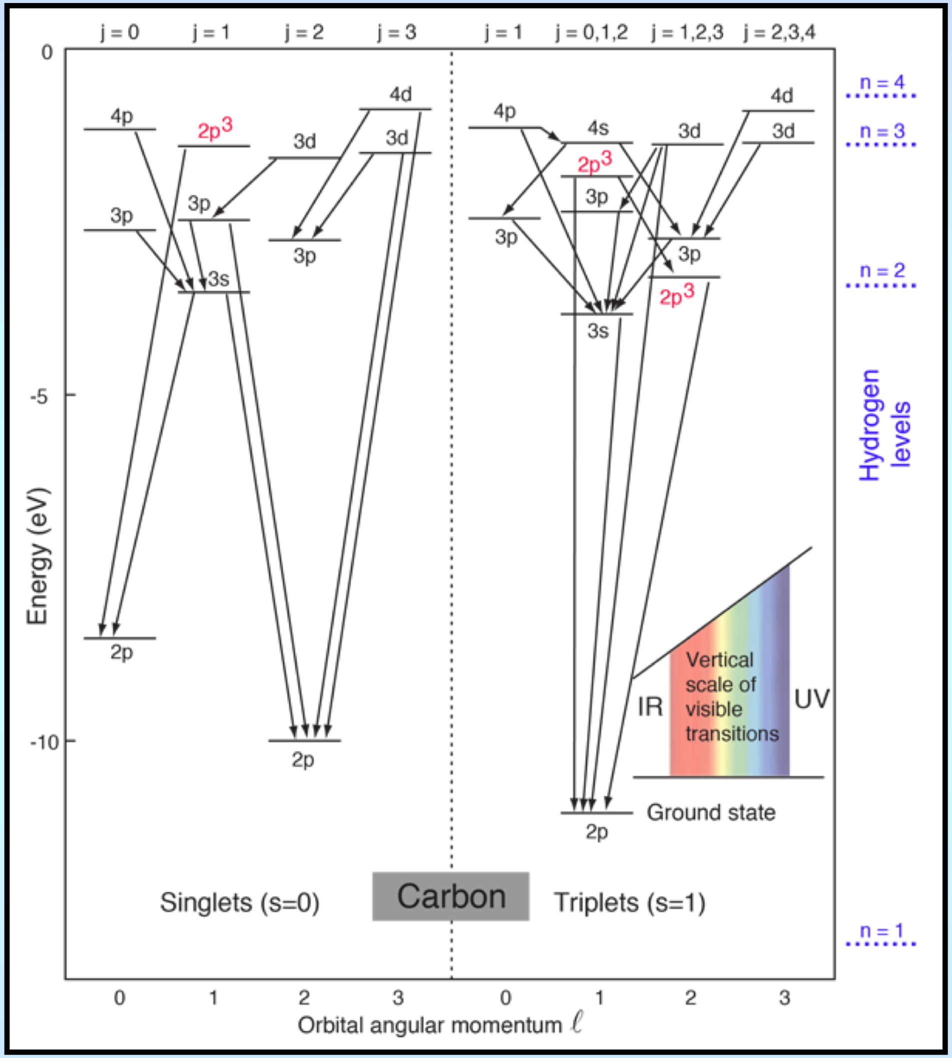
Forbidden transitions are noted by brackets, i.e., [O III] λ5007.



Atoms, Electrons, and Energy Levels

Atoms have many energy levels. In a high-density environment (such as this room), the atoms constantly collide with other, jostling the electrons around. The result is a Boltzmann distribution: if ω is a level's statistical weight and ΔE the difference between the energy levels, then the number of atoms in state i (n_i) compared to state j (n_j) is

$$\frac{n_i}{n_j} = \frac{\omega_i}{\omega_j} e^{-\Delta E/kT}$$

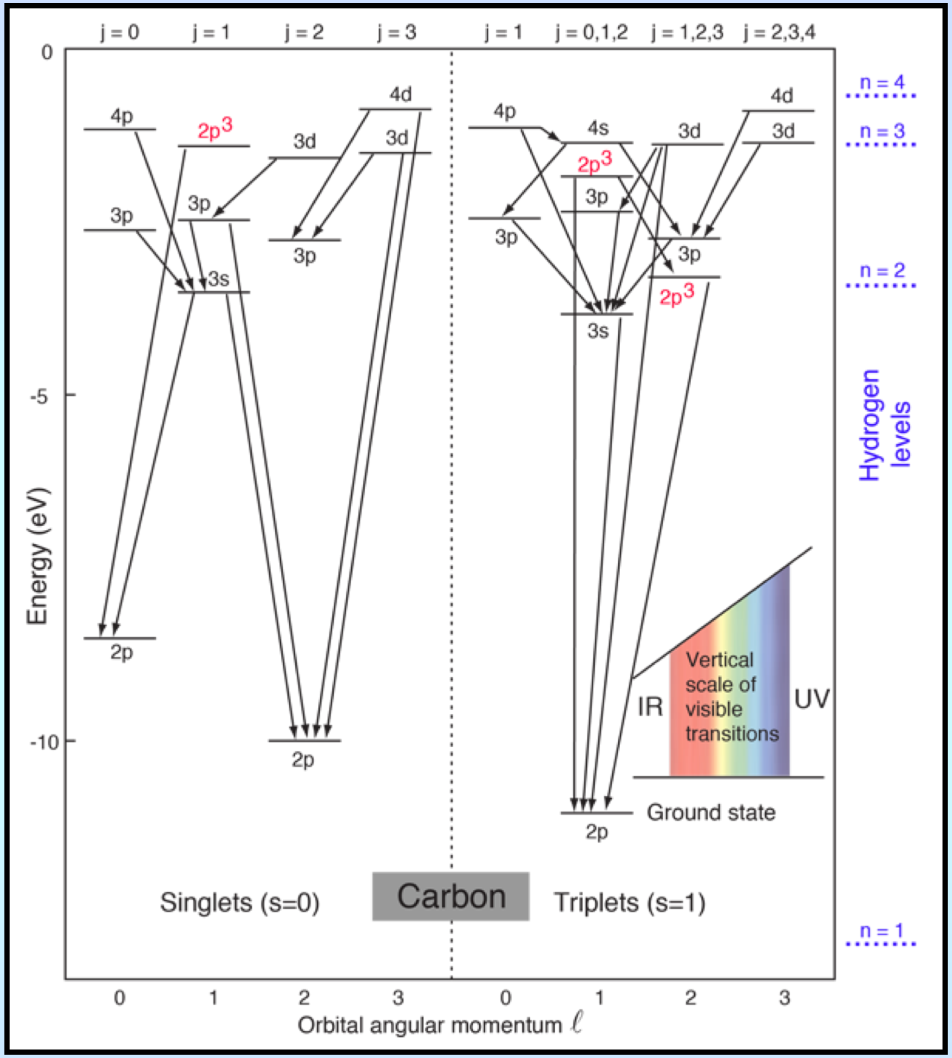


In this room, the electrons are in *thermodynamic equilibrium*.

Atoms, Electrons, and Energy Levels

In a low-density environment, the electrons have plenty of time to decay downward before a collision. In the case of the interstellar medium, virtually all the atoms will decay to their ground state long before a collision occurs.

In this case the electrons are not in thermodynamic equilibrium; the ground state will have far more electrons than the local "temperature" would suggest.



Source Material

Most of the details in this section come from **<u>the</u>** textbook on emission-line physics:

- Osterbrock (1974): **A**strophysics of **G**aseous **N**ebulae (affectionally known as AGN).

This book was re-printed and expanded in 1988 and became

- Osterbrock (1988): **A**strophysics of **G**aseous **N**ebulae and **A**ctive **G**alactic **N**uclei (a.k.a. AGN^2)

It was re-printed and expanded again in 2006 to

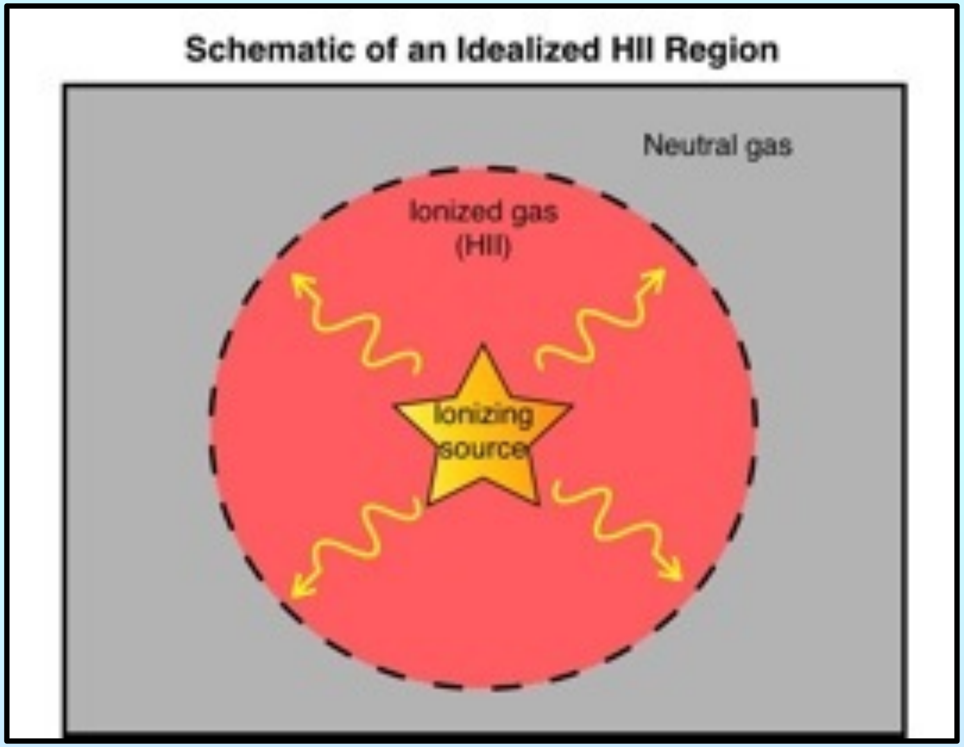
- Osterbrock & Ferland (2006): Astrophysics of Gaseous Nebulae and Active Galactic Nuclei (a.k.a. AGN^3)

There is also a *very* handy quick-reference chart in

Williams, R. 1995, Pub.A.S.P., 107, 152

The Warm Interstellar Medium

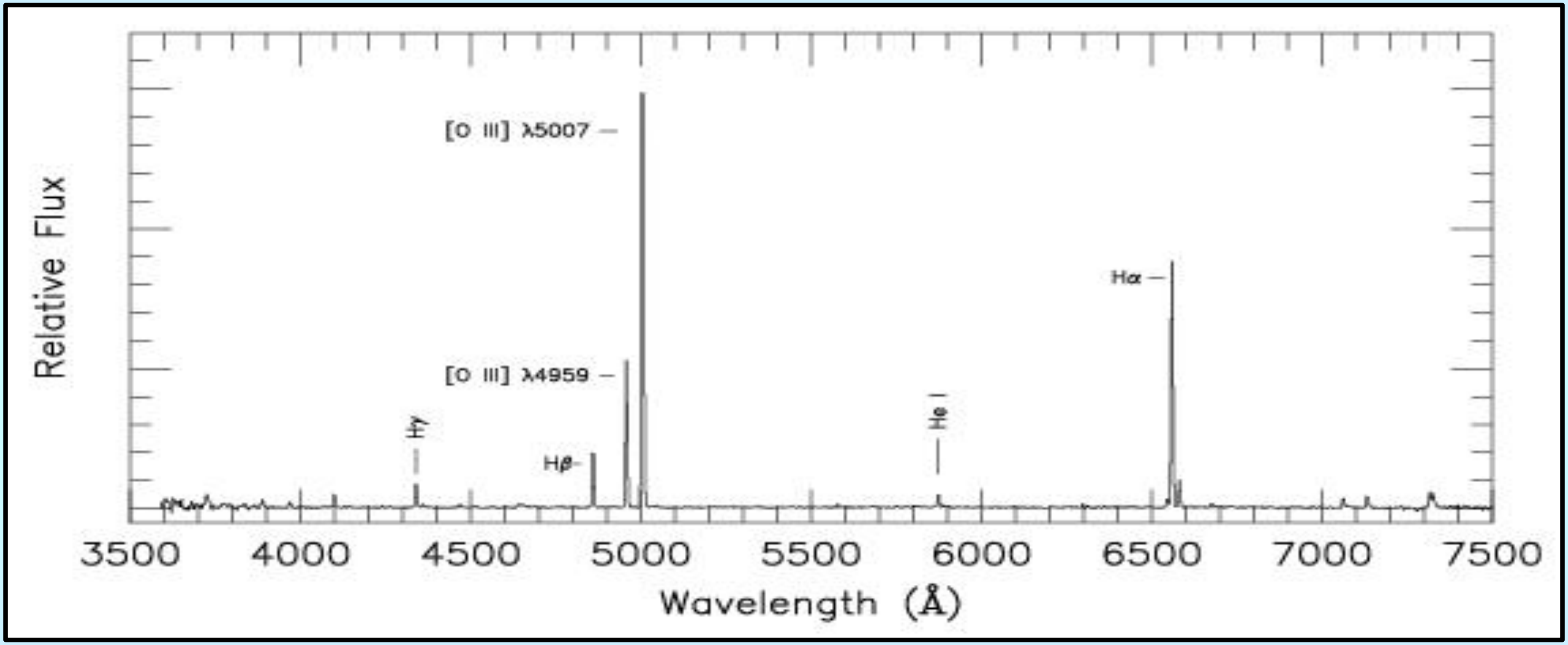
When you place a source of ionizing photons inside a region of neutral interstellar material, it creates a bubble of ionized material.



The spectrum of this region will contain many emission lines.

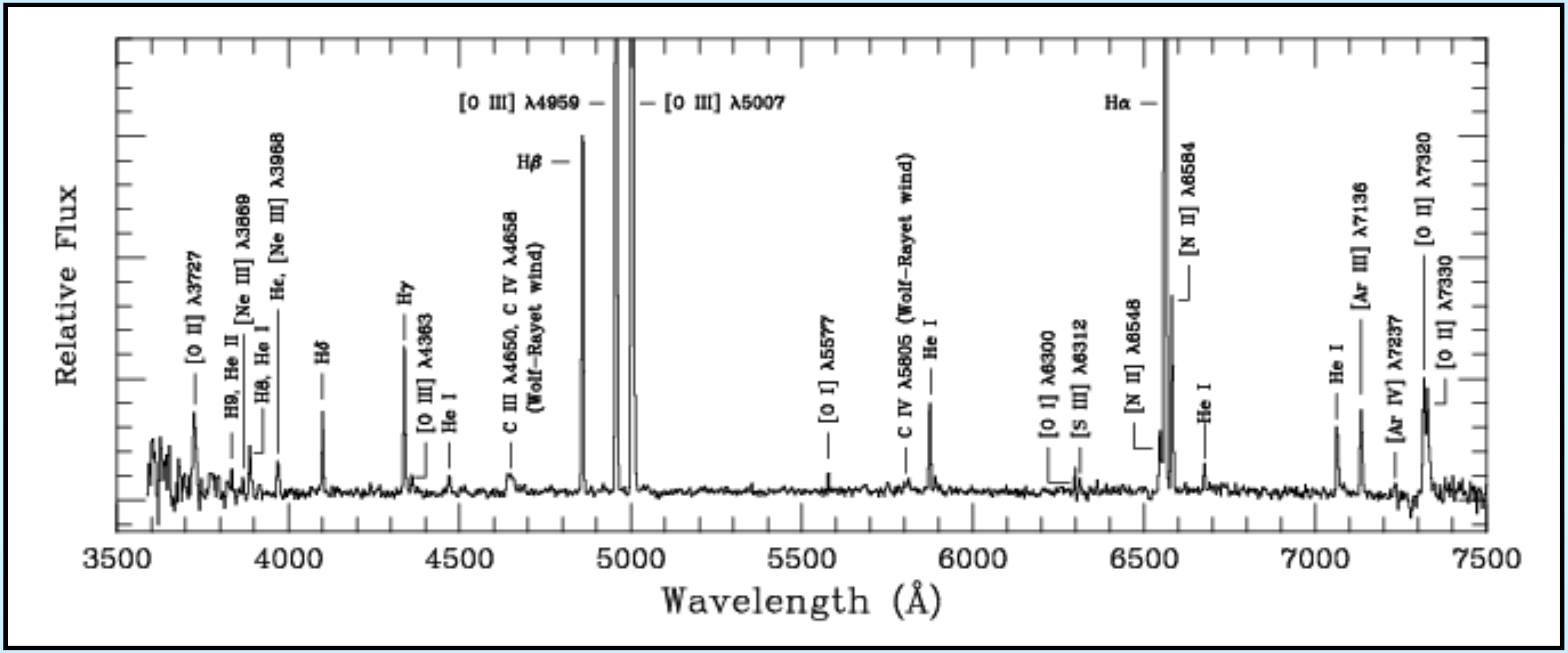
Goal: Explaining Emission Line Spectra

Area of ionized material may have a spectrum that looks like this:



Goal: Explaining Emission Line Spectra

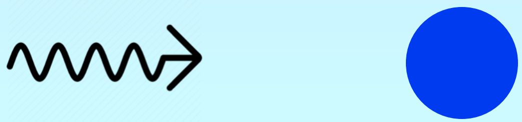
which, when expanded looks like



What determines the line strengths?

Hydrogen Ionization

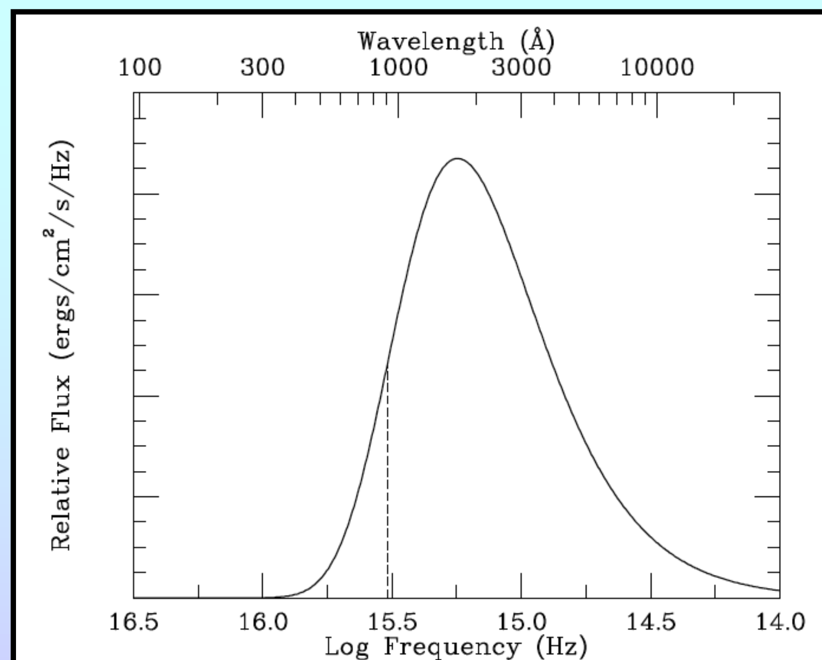
In the ISM, virtually all the hydrogen atoms are in their ground state. The cross-section for such an atom to a 13.6 eV photon is rather large; a 13.6 eV photon doesn't go far before hitting (and ionizing) a hydrogen.



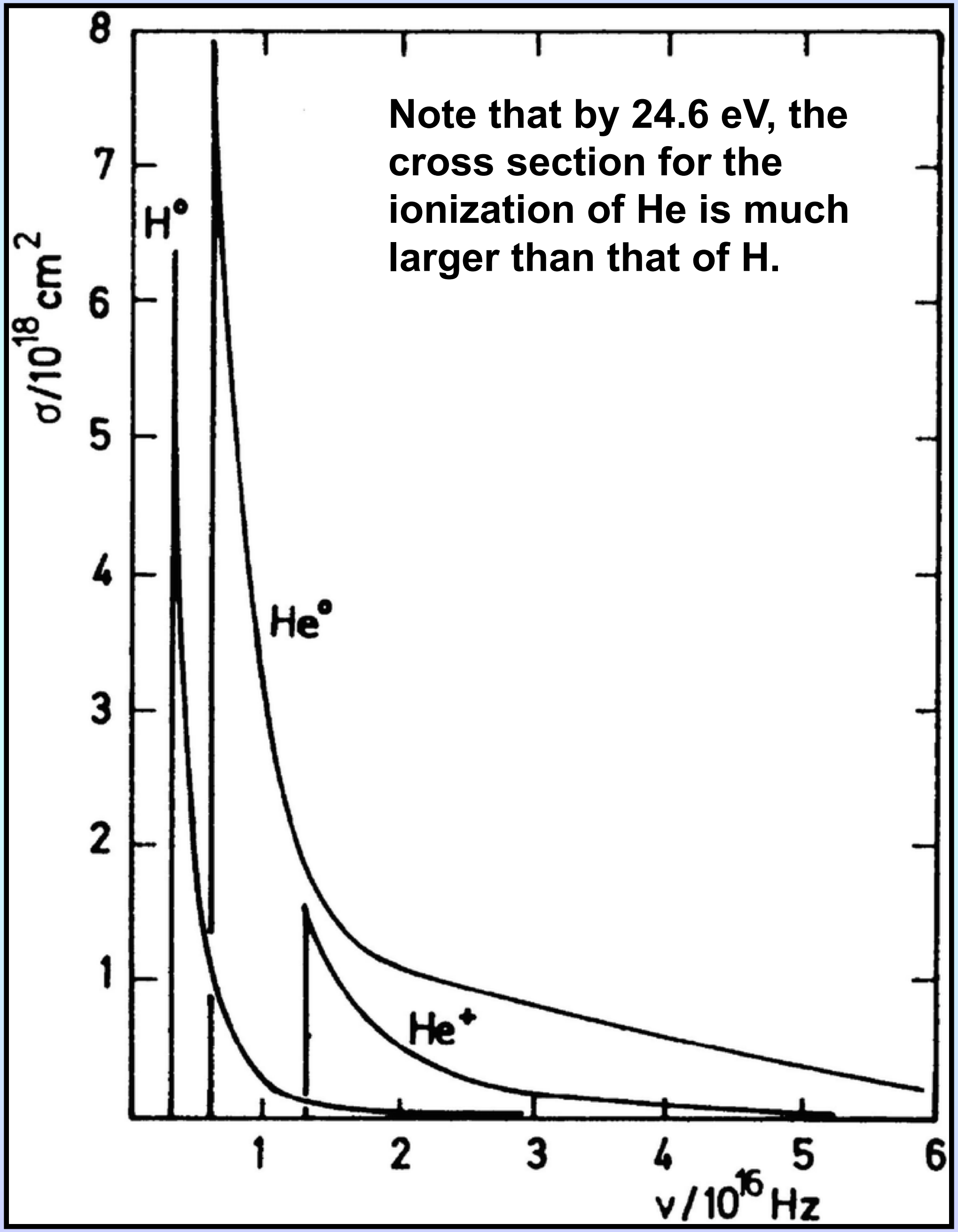
$$a = \pi\, r^2 = 6.30 \times 10^{-18}\ \mathrm{cm}^2$$

As the energy of the photon increases, the cross section decreases, with $a_\nu \propto 1/\nu^3$. (That's why there are a lot of x-ray astronomers, but very few far-UV astronomers!)

For most hot stars, the blackbody curve is declining rapidly shortward of 13.6 eV. Most of their ionizing photons are near 13.6 eV and very quickly absorbed.



Ionization of Other Species



Other ions behave the same way: the cross section for ionization is large at the ionization edge, then declines away roughly as $1/\nu^3$.

At the ionization edge of helium, the helium cross-section is ~ 6 times that of hydrogen.

At higher energies, it's the cross-section from heavy ions that provides the far-UV opacity.

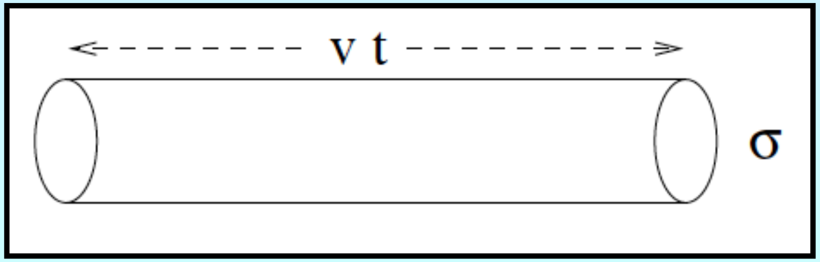
Ionization of Other Species

Element	II	III	IV	V
Hydrogen	13.6			
Helium	24.6	54.4		
Carbon	11.3	24.4	47.9	64.5
Nitrogen	14.5	29.6	47.4	77.7
Oxygen	13.6	35.1	54.9	77.4
Neon	21.6	41.0	63.5	97.1

Example: a typical O main sequence star will ionize hydrogen (and therefore oxygen), but it might not be hot enough to take the second electron off of oxygen.

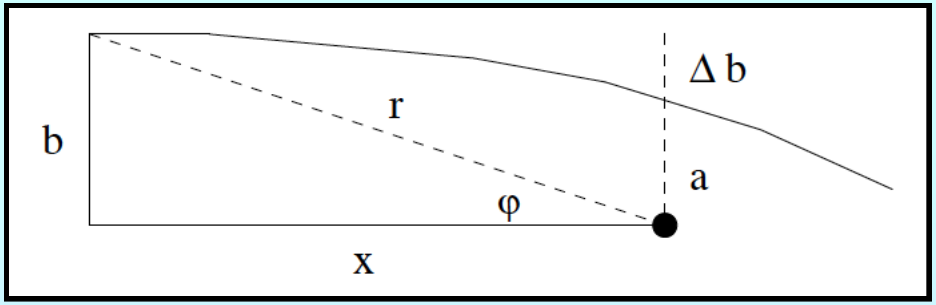
Recombination

Just as there was a cross-section for ionization, there is also a cross-section for the recombination of an electron into an atom. And like photo-ionizations, it depends on the energy (of the free electron).



Fast moving electrons cover more ground, and have more possible recombinations per second, $\alpha \propto v$.

Slow moving electrons give the electrostatic attraction more time to work, with $\alpha \propto 1/v^2$. (We'll prove this later.)



As a result, the recombination coefficient $\alpha = \sigma v \propto 1/v$. Since $v^2 \propto T$, that means that $\alpha \propto 1/\sqrt{T}$. For $T = 10{,}000°$, $\alpha_A = 4.18 \times 10^{-13}$ cm^3 s^{-1}, and the recombination rate is $R = N_e N_p \alpha_A$. (Note the subscript "A" on α; you'll soon see why it's there, and why α_A isn't often used.)

Typical Conditions

To get an idea of the state of the ISM near a source of high energy (E > 13.6 eV) photons, let's pick a spot ~ 5 pc from a 40,000° B-main sequence star. Let's also assume a typical ISM density of 1 particle cm^{-3}.

Since 9 out of 10 atoms in the universe is hydrogen, we'll make one further assumption (for now) that the nebula is entirely hydrogen. So N(H) = 1 cm^{-3}.

Question: How long will a hydrogen atom remain neutral?

The ionizing photon luminosity of a B main sequence star is

$$Q(H^0) = \int_{\nu_0}^{\infty} \frac{L_\nu}{h\nu} d\nu = 5 \times 10^{48} \text{ photons s}^{-1}$$

where ν_0 is the frequency for hydrogen ionization. At r = 5 pc from the star, the ionization rate is therefore

$$P = N(H^0) \int_{\nu_0}^{\infty} \frac{L_\nu}{4\pi r^2\, h\nu}\, a_\nu\, d\nu$$

In other words, the ionization rate is proportional to the density of neutral hydrogen atoms available for ionization, the flux of ionizing photons, and the cross-section for ionization. For 40,000° stars, the blackbody curve is dying rapidly shortward of 13.6 eV. So let's approximate a_ν as a constant, with $a_\nu \sim 5 \times 10^{-18}$ cm^2. Then

$$P \sim 10^{-8} \text{ ionizations cm}^{-3} \text{ s}^{-1}$$

So a hydrogen atom in a typical cm^3 of space will wait a year before being ionized.

Question: What is the distribution of states for Hydrogen?

The typical time is takes an atom to decay from state *nL* to state *n′L′* is simply the reciprocal of the Einstein A value. The typical time it takes to decay from state *nL* to any state is then

$$\tau_{nL} = \frac{1}{\displaystyle\sum_{n'<n} \sum_{L'=L\pm 1} A_{nL,n'L'}}$$

(By constraining $L' = L \pm 1$, we are neglecting forbidden transitions.) Typical permitted A values are $10^4 < A_{nl,n'L'} < 10^8$ sec^{-1}, so the timescale for decay is much less than a second. This is much less than the time between collisions (minutes to hours)! So all the hydrogen will be in the ground state.

[Esoteric note: hydrogen in the *n*=2 S state, has no permitted way to go to *n*=1 S. Electrons must either be a) collided out of the state, or b) decay via a low probability (A = 8.23 sec^{-1}) 2-photon emission. So rather than decaying down to the ground state is ~ 10^{-4} sec, these electrons will be hung up for $\tau = 0.12$ sec. More on this later.]

Question: Can Collisions Populate Hydrogen's n=2 State?

The energy difference between the ground state and first excited state of hydrogen is 10.2 eV, which corresponds to

$$E \sim \frac{1}{2} kT \quad \Longrightarrow \quad T \sim 80,000^\circ \ K$$

This is much hotter than the typical electron temperature in an ionized region (10,000° K). While electrons on the extreme tail of the Maxwellian curve might be able to excite an electron, this is rare. (And the electron would decay is much less than a second.)

Once a hydrogen electron reaches the ground state, it stays there.

Question: What Fraction of Hydrogen Atoms will be Neutral?

We have see that the rate of photo-ionizations

$$P = N(\mathrm{H}^0) \int_{\nu_0}^{\infty} \frac{L_\nu}{4\pi r^2\, h\nu} a_\nu \, d\nu \sim N(\mathrm{H}^0)\ 10^{-8}\ \mathrm{s}^{-1}$$

For steady state, the rate of photo-ionizations must equal the rate of recombinations. This rate is proportional to the density of free electrons, the density of free protons, and the recombination coefficient.

$$R = N_e N_p \, \alpha_A$$

where $\alpha_A \sim 4 \times 10^{-13}$ cm^3 s^{-1}. So ionization balance implies

$$N(\mathrm{H}^0) \int_{\nu_0}^{\infty} \frac{L_\nu}{4\pi r^2\, h\nu} a_\nu \, d\nu = N_e N_p \alpha_A$$

For pure hydrogen nebula, $N_e = N_p = (1 - \xi)\, N(\mathrm{H}^0)$, where ξ is the fraction of neutral material.

Ionization balance for pure hydrogen nebula then gives

$$N(\mathrm{H}^0)\int_{\nu_0}^{\infty}\frac{L_\nu}{4\pi r^2\,h\nu}a_\nu\,d\nu = N_e N_p \alpha_A$$

$$\xi N(\mathrm{H})\,\frac{(5\times 10^{48}\;\cdot\;5\times 10^{-18})}{3\times 10^{39}} = (1-\xi)^2 N(\mathrm{H})^2\;\cdot\;4\times 10^{-13}$$

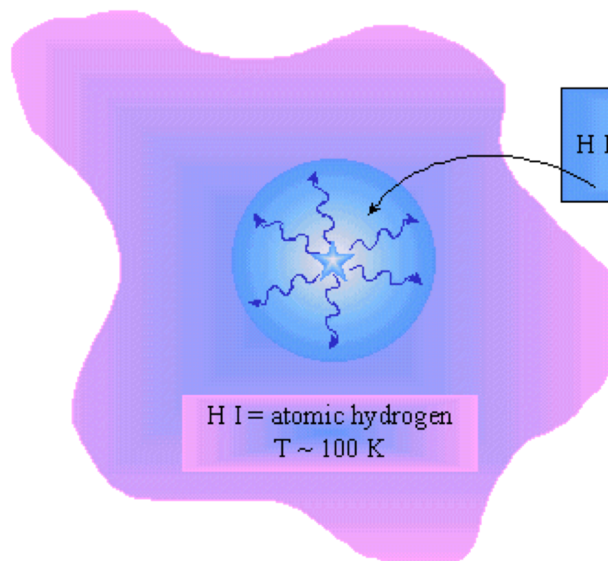
Solving for ξ with an ISM density of $N(H) \sim 1$ cm^{-3} yields an neutral fraction of $\xi = 4 \times 10^{-5}$. Virtually all the hydrogen is ionized!

Question: How thick is the transition region between the ionized and neutral material?

The mean free path of an ionizing photon is $\ell = \dfrac{1}{N(\mathrm{H}^0)a_\nu}$

The larger the cross section, or higher the density of neutral atoms, the shorter the path. By definition, in the transition region, half of the hydrogen is neutral, so $\ell = \left\{0.5\, N(\mathrm{H}^0)a_\nu\right\}^{-1}$

For photons near the ionization edge, $a_\nu \sim 5 \times 10^{-18}\,\mathrm{cm}^2$. Thus for a density of $N(\mathrm{H}) \sim 1$, $\ell \approx 4 \times 10^{17}$ cm, or ~ 0.1 pc. When the material starts to become neutral, the ionizing photons are rapidly eaten up. Considering that the entire H II region might be ~ 50 pc across, the transition region is very thin.

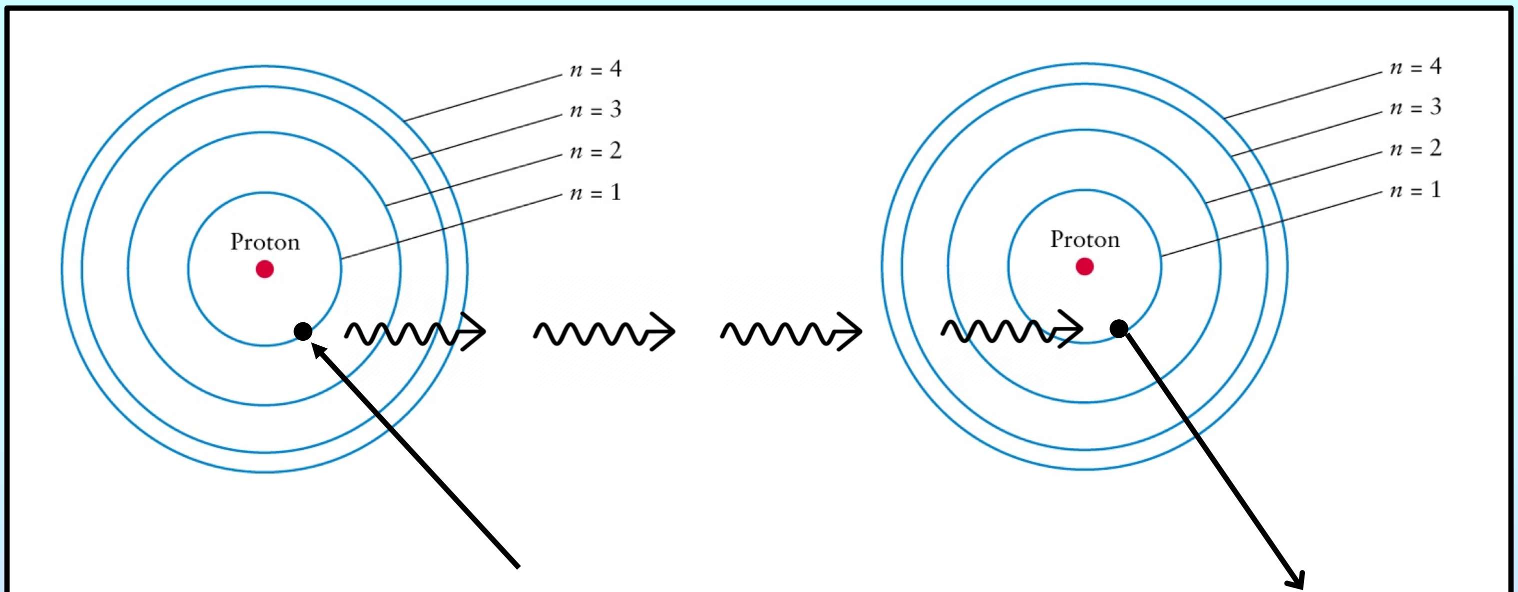


Unless the photon energies become really large, there is almost no transition region

Question: What is the Size of an Ionized Region?

There are 3 principles that govern the physics of an ionized region. The first is ionization balance: in steady state, the rate of photo-ionizations must equal the rate of recombinations.

The rate of photo-ionizations is proportional to the flux of ionizing photons, the density of neutral hydrogen atoms, and the cross-section for ionization. But not all ionizing photons come from the star!



Every recombination that goes directly into the ground state also produce an ionizing photon! That photon can then ionize a different hydrogen atom.

Ionization Balance

Because of this diffuse component of ionizing radiation, the equation of ionization balance is actually

$$N(\mathrm{H}^0) \int_{\nu_0}^{\infty} \frac{4\pi J_\nu}{h\nu} a_\nu \, d\nu = N_e N_p \alpha_A$$

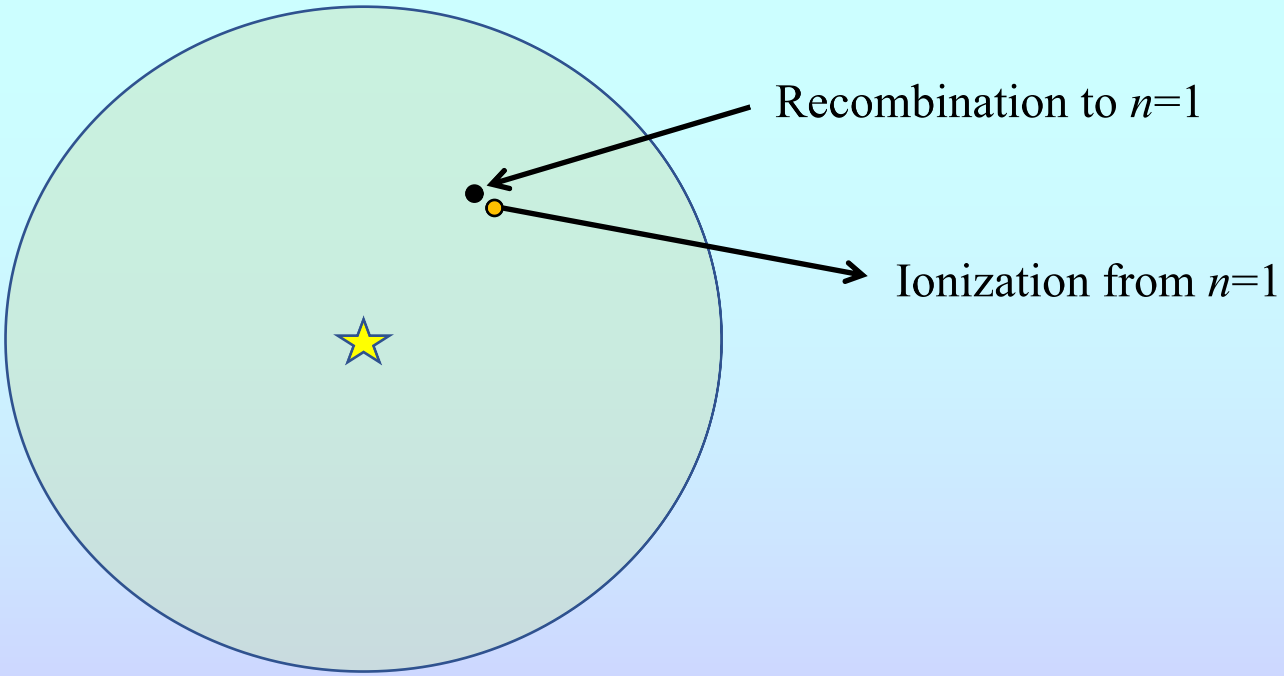
where J_ν is the mean intensity of radiation, in units of energy per unit area, per unit time, per unit frequency, per unit solid angle. (The 4π term is the implicit integration over all directions.) Note that J_ν has two components: the ionizing radiation from the central star, and the diffuse component.

Fortunately, most recombinations that produce the diffuse component come from slow-moving electrons (due to the electrostatic focusing). Thus, $\nu \approx \nu_0$, and the cross-section for re-absorption is very high. So there's a way to simplify the problem.

Question: What is the Size of an Ionized Region?

Suppose we make the "on the spot" approximation and say that every recombination directly to the ground state ionizes a hydrogen atom that is *very* nearby. In that case, it's like nothing happened!! This assumption is equivalent to saying

- All ionizing photons come from the central ionizing source
- Recombinations directly to the ground state do not occur.



Ionization Balance

Under the on-the-spot approximation, ionization balance becomes

$$N(\mathrm{H}^0)\int_{\nu_0}^{\infty}\frac{L_\nu}{h\nu}a_\nu\,e^{-\tau_\nu}\,d\nu = 4\pi r^2 N_e N_p \alpha_B$$

where α_B is the recombination rate to all levels *except* the ground state. For a 10,000° plasma, $\alpha_B = 2.59 \times 10^{-13}$ cm^3 s^{-1}. The optical depth, τ_ν, is

$$\tau_\nu(r) = \int_0^r N(\mathrm{H}^0)\,r'a_\nu\,dr'$$

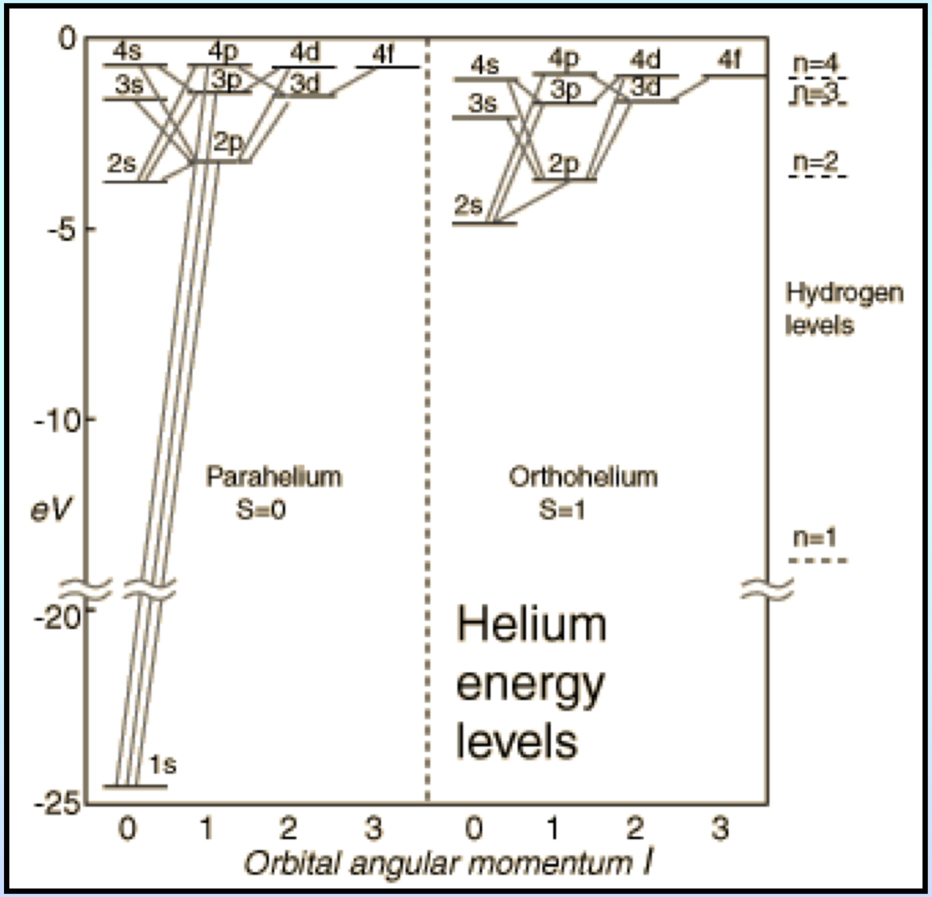
For a constant density nebula, these two equations can be integrated to give the radius, $\mathcal{R}$, of the nebula as a function of the density and the number of ionizing photons/sec being produced by the star

$$Q(\mathrm{H}^0) = \int_{\nu_0}^{\infty}\frac{L_\nu}{h\nu}d\nu = \int_0^{\mathcal{R}} N_e N_p \alpha_B dV = \frac{4}{3}\pi\mathcal{R}^3 N(\mathrm{H})^2\alpha_B$$

The ionized region is called the Strömgren sphere.

Notes on Ionization Balance

- The previous analysis assumed a pure hydrogen nebula. But the existence of helium doesn't really make a difference. Yes, some photons ionize helium instead of hydrogen but they are returned.



The difference between the ground state and the n=2 states of helium are so great that all helium recombinations will eventually create a photon that is capable of ionizing hydrogen.

Notes on Ionization Balance

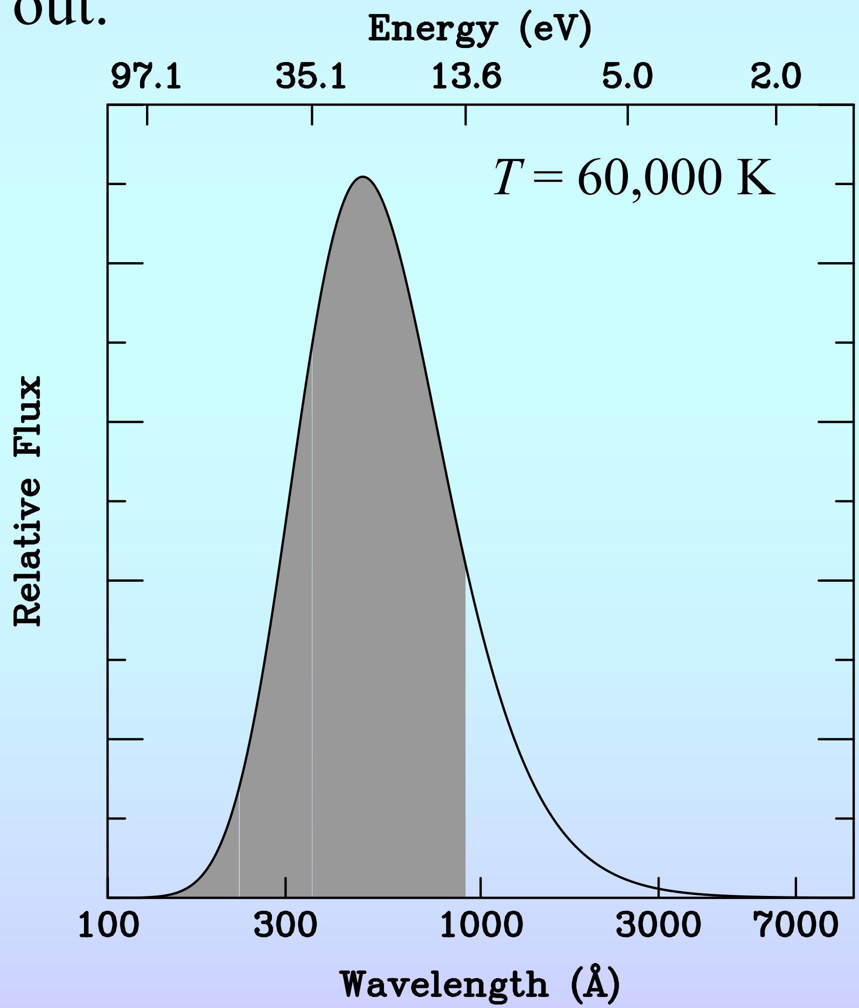
- The previous analysis assumed a pure hydrogen nebula. But the existence of helium doesn't really make a difference. Yes, some photons ionize helium instead of hydrogen but they are returned.
- The "on-the-spot" approximation can fail if the density becomes very low, since $\ell = \left\{0.5\, N(\mathrm{H}^0) a_\nu \right\}^{-1}$. But it is usually a good assumption (and it simplifies calculations enormously). In almost all cases α_B is used instead of α_A.
- Nine of out 10 atoms in the universe are hydrogen. Seven out of 10 of what's left is helium. So the heavier elements do not make any difference to the nebula's ionization balance.

Energy Balance

The second principal that governs ionized regions is energy balance. The energy deposited into a region (via photo-ionizations) resides in its free electrons. But that energy must eventually be re-emitted: energy in equals energy out.

Because of their high ionization cross-section, the energy contained in all of the photons shortward of 13.6 eV is trapped. The free electrons have this energy.

For hot stars, this is most of their luminosity! This trapped energy can't stay there forever. The energy gained (G) must equal the energy lost (L).



Heating the ISM

To apply energy balance, first consider the initial energy of the free electrons. Every ionization creates a free electron with

$$\frac{1}{2} m_e v^2 = h(\nu - \nu_0)$$

The total heating from hydrogen ionization is then

$$G(\mathrm{H}) = N(\mathrm{H}^0) = \int_{\nu_0}^{\infty} \frac{4\pi J_\nu}{h\nu} h(\nu - \nu_0) d\nu$$

which through ionization balance is

$$G(\mathrm{H}) = N_e N_p \alpha_A \frac{\displaystyle\int_{\nu_0}^{\infty} \frac{4\pi J_\nu}{h\nu} h(\nu - \nu_0) d\nu}{\displaystyle\int_{\nu_0}^{\infty} \frac{J_\nu}{h\nu} a_\nu d\nu}$$

There are similar equations for the heating helium and ionized helium, so $G = G(\mathrm{H}^0) + G(\mathrm{He}^0) + G(\mathrm{He}^+)$. Other elements are so rare that they are irrelevant to the heating.

Energy Balance

Most of the energy that goes into ionization comes out via 3 mechanisms:

- Thermal Bremsstrahlung (free-free emission): free electrons have their paths distorted by the attraction/repulsion of other charged particles. When this happens, they emit light.

$$L_{\mathrm{ff}} = \frac{2^5 \pi e^6 Z^2}{3^{\frac{3}{2}} h m_e c^3} \left(\frac{2\pi k}{m_e} \right)^{1/2} T_e^{1/2} g_{\mathrm{ff}} N_e N_+$$

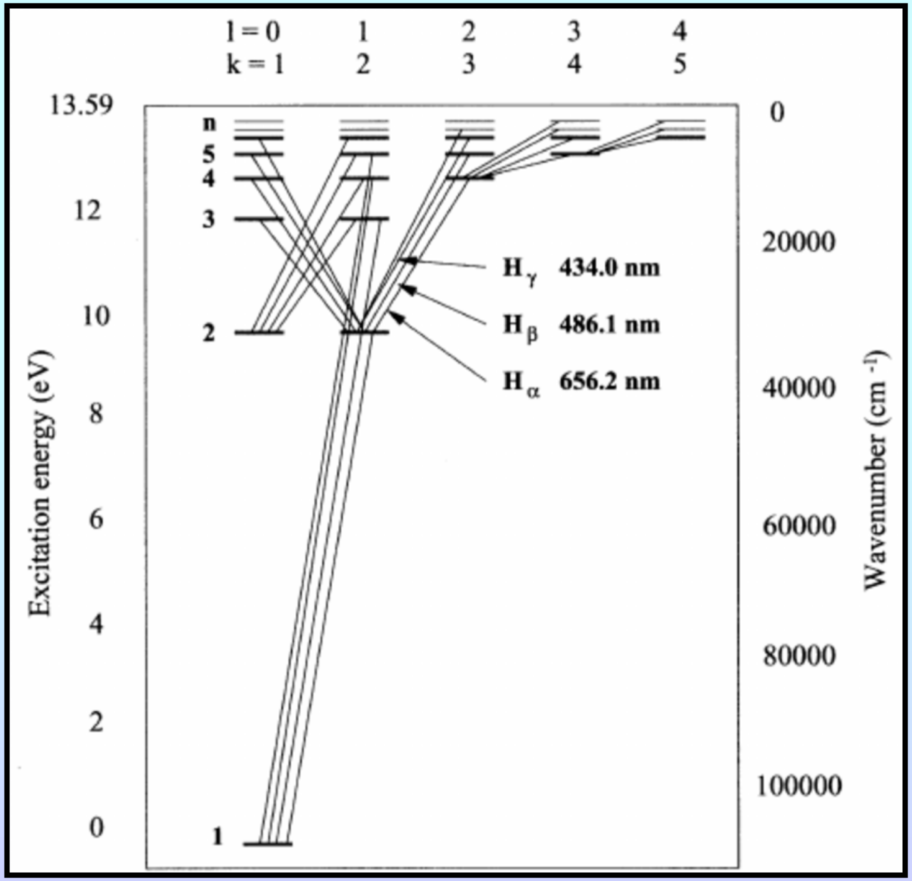
$$= 1.42 \times 10^{-27} Z^2 T_e^{1/2} N_e N_+ \text{ ergs cm}^{-3}\text{s}^{-1}$$

This mechanism pops up a lot in astrophysics, but for regions of ionized gas, its effect is minor. The light comes out at all wavelengths, but for most ionized regions, it is easiest to observe in the radio. In general, this mechanism is wimpy: relatively little energy is emitted via free-free emission.

Energy Balance

Most of the energy that goes into ionization comes out via 3 mechanisms:

- Thermal Bremsstrahlung (free-free emission): free electrons have their paths distorted by the attraction/repulsion of other charged particles. When this happens, they emit light.
- Recombination: electrons recombine into their atoms and cascade down, creating a series of emission lines.



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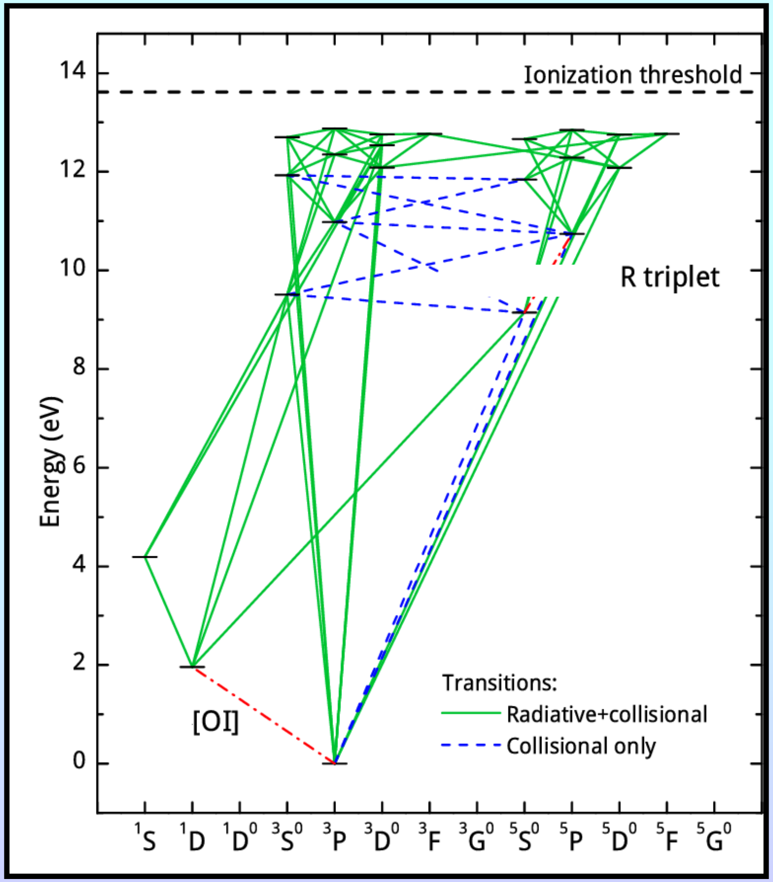
- Thermal Bremsstrahlung (free-free emission): free electrons have their paths distorted by the attraction/repulsion of other charged particles. When this happens, they emit light.
- Recombination: electrons recombine into their atoms and cascade down, creating a series of emission lines.
- Collisional excitation: a free electrons collides with a (ground-state) electron within an atom. The bound electron is pushed to a higher level; when it falls back down, it emits the energy.



Notes on Recombinational Cooling

Cooling by recombination is generally expressed via the kinetic-energy weighted recombination coefficient to each level of the atom

$$L_R(\mathrm{H}) = N_e N_p k T_e \beta_A \quad \text{where} \quad \beta_A = \sum_{n=1}^{\infty} \sum_{L=0}^{n-1} \beta_{n,L}$$

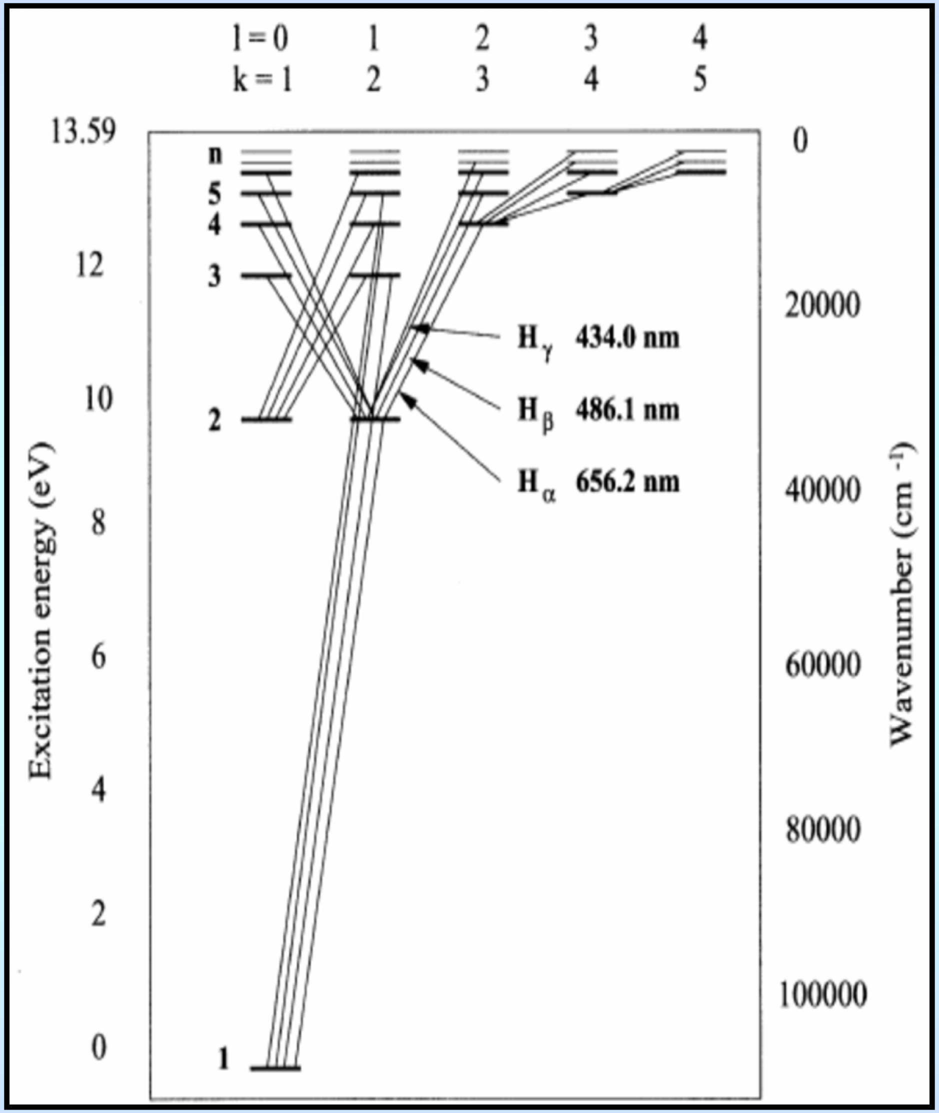
The units of β_A are similar to that of the recombination coefficient, cm^3 s^{-1}. So in the cooling expression, kT_e gives L_R units of energy. A typical value for β is 10^{-13} cm^3 s^{-1}. There are similar equations for helium.

Note: as we saw, electrostatic focusing causes slow moving electrons to be more likely to recombine than fast moving electrons. If L_R were the only source of nebular cooling, the electron temperature would actually increase! This same effect makes the on-the-spot approximation for thermal balance less accurate than it is for ionization balance. (The slow moving electrons from the diffuse field are more important.) So β_A is used more often than β_B.

Notes on Collisional Excitation

Virtually all the atoms in the ISM are in their ground state. Since the free electrons in the ISM have a finite temperature, the likelihood of a collisional excitation depends on how reachable the next level is.

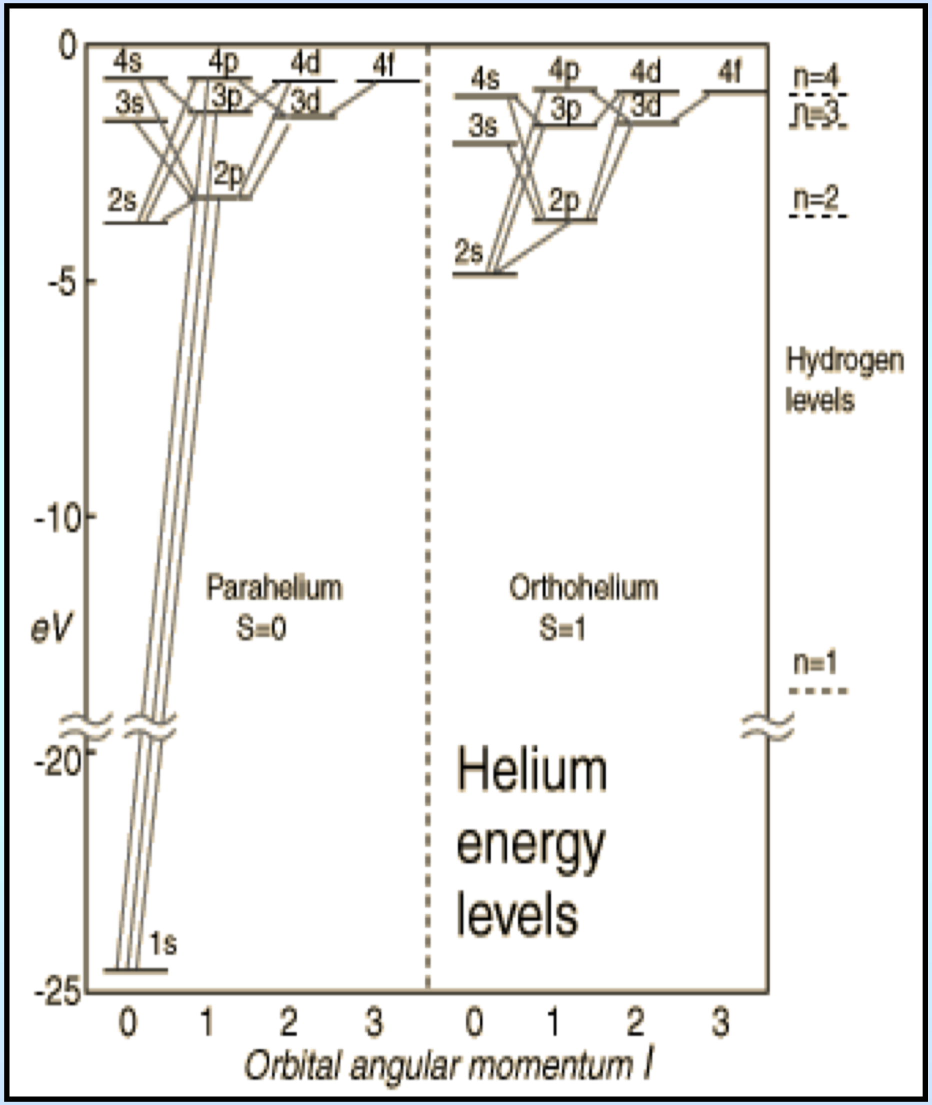
For hydrogen, the lowest excited level is 10.2 eV above the ground state. That is much greater than the ~1 or 2 eV energies of the free electrons. Collisional excitation of hydrogen is *rare*.



Notes on Collisional Excitation

Virtually all the atoms in the ISM are in their ground state. Since the free electrons in the ISM have a finite temperature, the likelihood of a collisional excitation depends on how reachable the next level is.

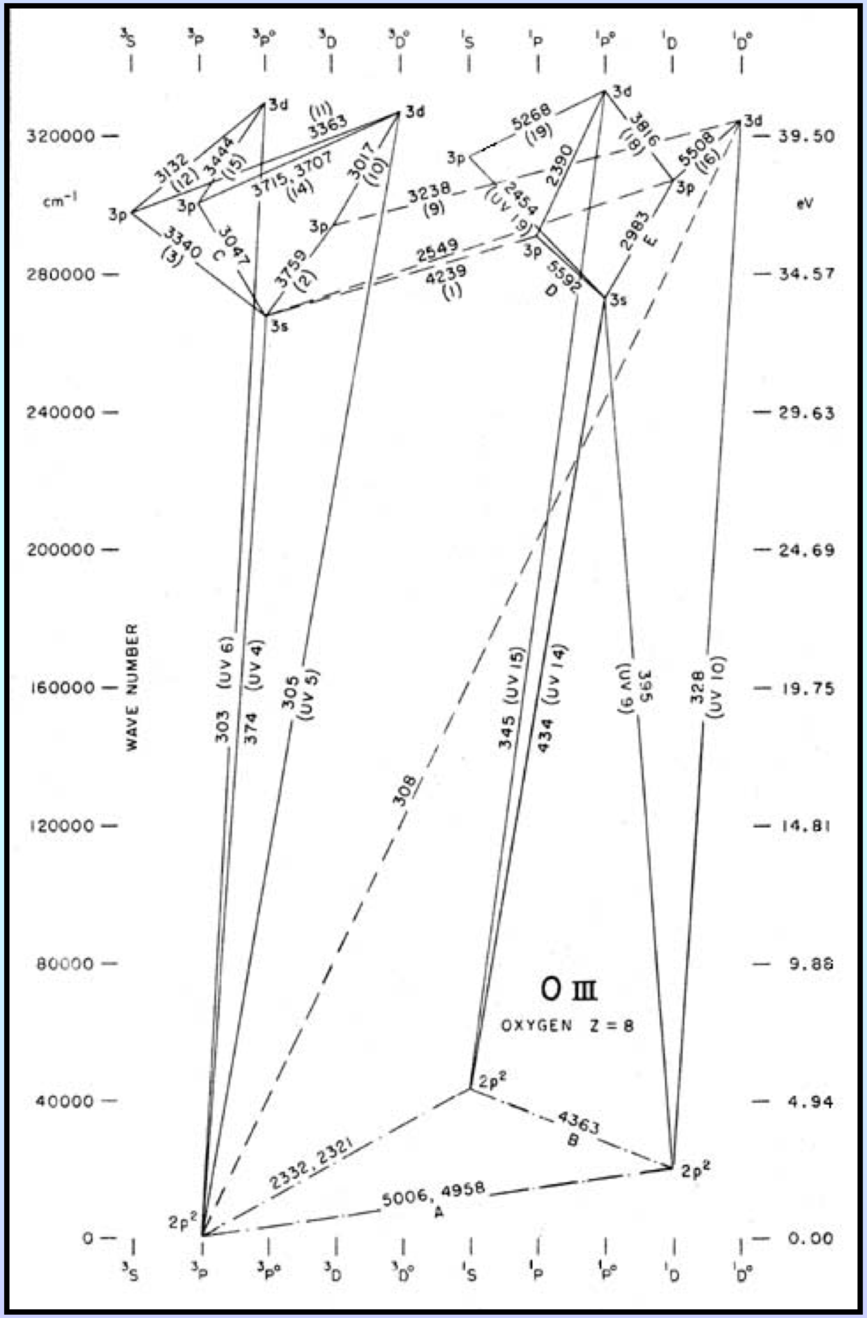
For helium, the lowest excited level is ~ 19.75 eV above the ground state. The free electrons do not have anywhere near this amount of energy.



Notes on Collisional Excitation

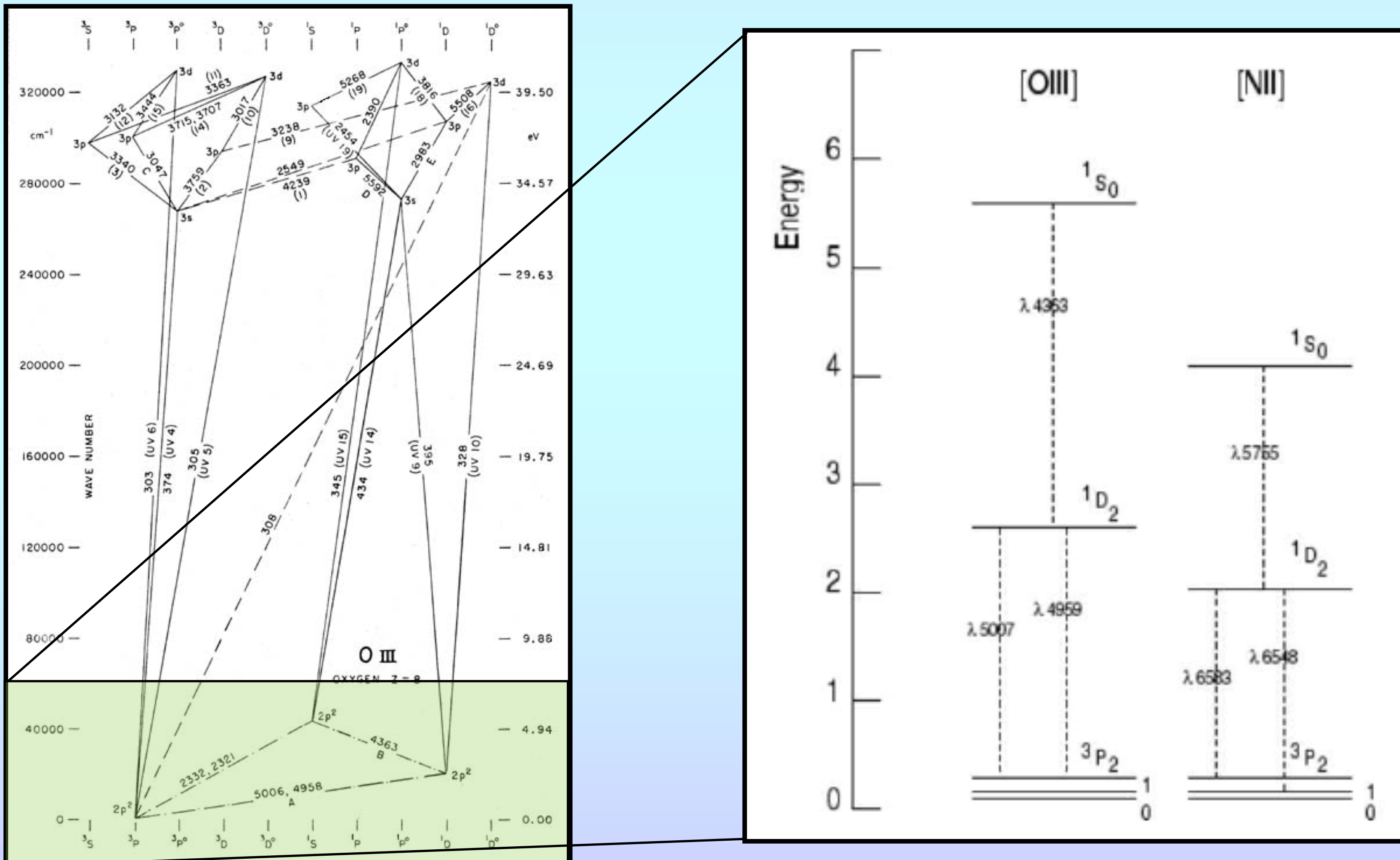
Virtually all the atoms in the ISM are in their ground state. Since the free electrons in the ISM have a finite temperature, the likelihood of a collisional excitation depends on how reachable the next level is.

The best species for collisional excitation are (relatively common) atoms/ions that have 2, 3, or 4 electrons in the outer p-orbital. In other words, C, N, O, Ne, S, and Ar.



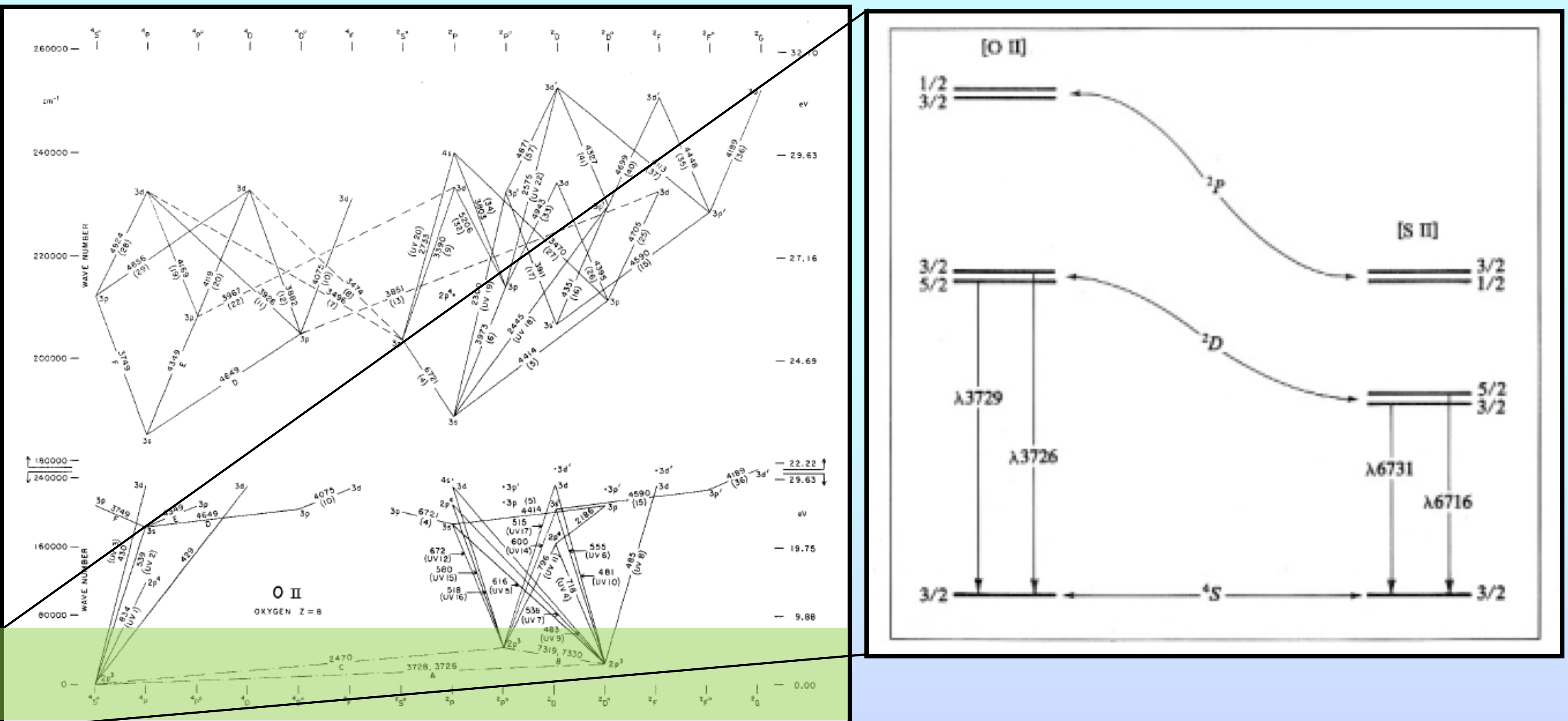
Isoelectronic Species

All species with 2 or 4 electrons in the outer p-shell have the same configuration of low-lying energy levels, i.e., 3-1-1. These species include C^0, N^+, O^{++}, Ne^{+4}, S^{++} and Ar^{+4}, O^0, and Ne^{++}.



Isoelectronic Species

All species with 3 electrons in the outer p-shell have the same configuration of low-lying energy levels, i.e., 2-2-1. These species include N^0, O^+, Ne^{+3}, S^+ and Ar^{+3}.



Collisional Excitation

In general, the rate of collisions from state i to state j ($q_{i,j}$) depends on

- The density of free electrons, $q_{i,j} \propto N_\mathrm{e}$
- The density of the target species, $q_{i,j} \propto N_\mathrm{X}$
- a term for the volume being swept out by a free electron each second ($\sigma \propto v$) and the effects of electrostatic focusing ($\sigma \propto v^{-2}$). In terms of temperature, this means $q_{i,j} \propto 1/\sqrt{T_e}$
- The energy difference between where the bound electron starts (level i) and where it ends up (level j). If $\Delta E_{i,j}$ is large, only a small fraction of the free electrons will have the energy to cause an excitation, so $q_{i,j} \propto e^{-\Delta E/kT_\mathrm{e}}$ if $\Delta E > 0$.
- The statistical weight of the level the bound electron begins in, ω_i.
- Some term (of the order unity) that contains all the quantum mechanical nastiness associated with the overlapping wave function during the collision, $\Omega_{i,j}$.

Collisional Excitation

Put this all together, and the collisional cooling going from state *i* to state *j* for any species is

$$L_c = N_e N_i q_{i,j} \;\cdot\; \Delta E_{i,j} \quad \text{where}$$

$$q_{i,j} = \left(\frac{2\pi}{kT_e}\right)^{1/2} \frac{\hbar}{m_e^{3/2}} \frac{\Omega_{i,j}}{\omega_i}\, e^{-\Delta E_{i,j}/kT_e}$$

$$= 8.629 \times 10^{-6} \frac{\Omega_{i,j}}{\omega_i T_e^{1/2}}\, e^{-\Delta E_{i,j}/kT_e} \ \text{cm}^3\ \text{s}^{-1}$$

Though it is rare in the ISM, collisions can also cause electrons to go from an upper level to a lower level. In that case, the equation is the same and $\Omega_{i,j} = \Omega_{j,i}$, but the cooling is negative and there is no exponential Boltzmann factor (since all free electrons are capable of doing this).

Notes on Ω

- The quantum mechanical collisional strength is symmetrical, with $\Omega_{i,j} = \Omega_{j,i}$. Consequently,

$$q_{i,j} = \frac{\omega_j}{\omega_i} e^{-\Delta E/kT_e}\, q_{j,i}$$

- If either S = 0 or L = 0 for a level, then there's a simple relation for the collision strength between a term with a singlet level and a term containing several levels, i.e.,

$$\Omega(SLJ, S'L'J') = \frac{(2J'+1)}{(2S'+1)(2L'+1)} \Omega(SL, S'L')$$

Collisional Cooling

If every collisional excitation from the ground state of species X to level j were followed (eventually) by a decay (or decays) back to the ground state, then the emitted photons which leave the nebular will carry away

$$L_C = N_e N_X q_{1,j} \; \cdot \; h\nu_{1,j}$$

But in practice, collisional de-excitation can also occur. Consider a two-level atom. If N_1 is the number of atoms in the ground state, and N_2 is the number of atoms in the excited state, then in equilibrium

$$N_e N_1 q_{1,2} = N_e N_2 \, q_{2,1} + N_2 A_{2,1}$$

The relative level population is therefore

$$\left(\frac{N_2}{N_1} \right) = \frac{N_e q_{1,2}}{N_e q_{2,1} + A_{2,1}}$$

The collisional cooling rate for this two-level ion is therefore

$$L_C = N_2 A_{2,1}\, h\nu_{2,1} = \frac{N_1 N_e q_{1,2}}{N_e q_{2,1} + A_{2,1}} A_{2,1}\, h\nu_{2,1}$$

or

$$L_C = N_1 N_e q_{1,2}\, h\nu_{2,1} \left\{ \frac{1}{\frac{N_e q_{2,1}}{A_{2,1}} + 1} \right\}$$

Note the limits:

$$N_e \to 0, \quad L_C = N_1 N_e\, q_{2,1}\, h\nu_{2,1}$$

$$N_e \to \infty,\, L_C = N_1 \left(\frac{q_{1,2}}{q_{2,1}} \right) A_{2,1}\, h\nu_{2,1} = N_1 \left(\frac{\omega_2}{\omega_1} \right) e^{-\Delta E/kT_e} A_{2,1}\, h\nu_{2,1}$$

In the low density limit, the cooling is proportional to the electron density, and every collision upward creates a photon which cools the nebula. At high densities, the cooling rate equals that for a gas in thermodynamic equilibrium and doesn't depend on electron density.

Final Notes on Energy Balance

Collisional cooling is always most efficient for ions where $\Delta E \approx kT_e$. If $\Delta E \gg kT_e$, then very few electrons will be excited, so little cooling will occur; if $\Delta E \ll kT_e$, then the amount of energy released in the downward transition will be inconsequential.

Energy balance in an ionized nebula is simply

$$G(\mathrm{H}^0) + G(\mathrm{He}^0) + G(\mathrm{He}^+) = L_{\mathrm{ff}} + L_R + L_C$$

In this equation, $G(\mathrm{H}^0)$ and L_C are by far the most important.

In the low density limit, each term is proportional to electron density, so N_e has no effect on energy balance and the nebular temperature will only depend on the energy of the ionizing photons and on the ionic abundances. At high densities, however, collisional de-excitations will decrease the efficiency of collisional cooling. Therefore, all things being equal, denser nebulae will be hotter.